Institute for Mathematics and its Applications

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IMA NEWSLETTER # 251

June 1–30, 1997

1996–97 Program

MATHEMATICS IN HIGH-PERFORMANCE COMPUTING

See the Winter, Summer and Fall 1996 IMA Update for a full description of the 1996–97 program on Mathematics in High-Performance Computing.

News and Notes

IMA Workshop:

Parallel Solution of PDE

June 9–13, 1997
Organizers: Mitchell Luskin (University of Minnesota) and Petter Bjørstad (University of Bergen)

Workshop on Automatic Differentiation for Large-Scale Applications

The IMA will hold a special workshop on **Template-Driven Automatic Differentiation for Large-Scale Scientific and Engineering Applications** June 29–July 3, 1997, organized by Thomas Coleman (Cornell), Fadil Santosa (Minnesota) and William Symes (Rice). The IMA, the Cornell Theory Center and CRPC at Rice University are joint sponsors. The full workshop description and schedule will appear in the July, 1997 IMA Newsletter.

The workshop will bring together researchers from a variety of fields interested in applications of AD to contemporary scientific and engineering problems of very large scale, *e.g.* inverse problems and optimal design, to explore the benefits of algorithmic decomposition. It will also involve AD package authors, who will offer their insights and expertise in design and application of AD and perhaps take away some revised goals for AD research. Participants will be invited to bring code of current interest and will apply various AD tools during the workshop, reporting results in seminar as the week progresses.

Dynamical Systems Postdocs Selected

With the advice of the organizers of the 1997–98 year on **Emerging Applications of Dynamical Systems,** the IMA has chosen nine postdoctoral members for the period September 1, 1997 to August 31, 1998. These postdocs will be active participants in all activities of the Dynamical Systems year. They were chosen from a long list of well-qualified recent Ph. D. recipients.

NAME	PH. D. INSTITUTION	DATE	ADVISOR
Miaohua Jiang	Georgia Inst. of Technology	1995	Yakov Pesin
Mark Johnson	Princeton University	1997	Yannis Kevrekidis
Rolf-Martin Mantel	University of Warwick	1997	Dwight Barkley
Kurt Lust	Catholic Univ. of Leuven	1997	Dirk Roose
Ricardo Oliva	Cornell University	1997	John Smillie
Kathleen Rogers	University of Maryland	1997	John Maddocks
Tony Shardlow	Stanford University	1997	Andrew Stuart
Shinya Watanabe	Massachusetts Inst. of Technology	1995	Steven Strogatz
Warren Weckesser	Rensselaer Polytechnic Inst.	1997	Mark Levi

Participating Institution Conferences Selected for 1997–98

Seven IMA Participating Institution Conferences have been selected for funding during 1997–98:

DATES	LOCATION	TITLE
June 1-3, 1997	Indiana University	Nonlinear Problems in the Applied Sciences
July 30–August 3, 1997	Penn State University	Topics in Number Theory
December 14–16, 1997	Univ. of Southern California	Stochastic Control and Nonlinear Filtering
March 25–28, 1998	University of Cincinnati	Global Analysis 30 Years Later
Spring 1998, date TBA	Purdue University	Workshop on Superconductivity
June 3–6, 1998	Univ. of Wisconsin-Madison	7th Conference of the International Linear Algebra Society
September 26–28, 1998	University of Pittsburgh	Waves and Continuation Methods in Biology and Related Areas

Interested participants are urged to address their inquiries to the organizers at the Participating Institution where the conference will be held. Conference Participants from other Participating Institutions may use PI funds for their expenses, where these are available.

All faculty members of Participating Institutions of the IMA were encouraged to submit proposals for this annual competition. There is no restriction on the mathematical topic of the conferences, but they should be of interest to a number of Participating Institutions, and the organizing committee should contain some faculty members from these institutions. The faculties of the Participating Institutions were consulted about the proposals, and the final decision was made by a panel of four participating Institution department heads: Peter Hislop (University of Kentucky)(chair), Shui-Nee Chow (Georgia Tech), Bill Rundell (Texas A&M University), and Boris Rozovskii (University of Southern California). Proposals for 1998–99 will be due in April, 1998.

Improved IMA Home Page

The IMA has substantially improved its home page on the World-Wide Web, accessible through netscape or other web-reading applications at

`http://www.ima.umn.edu.`

The page is continually under construction. We invite comments or suggestions, which may be addressed to

`webmaster@ima.umn.edu.`

In particular, we appreciate any information about World-Wide Web links appropriate to current and upcoming IMA programs.

Schedule for June 1–30, 1997

Monday, June 2

Tuesday, June 3

IMA Postdoc Seminar

2:30 pm	**Rosemary Renaut** Arizona State University	Parallel Multisplitting Applied for Solution of the Least-Squares Problem

Abstract: The single-splitting idea, in its simplest form usually seen as a Jacobi or Gauss-Seidel iteration, can be generalised by means of a multi-splitting (MS) to provide iterative methods suitable for parallel architectures. I shall review the notion of multisplitting, in particular considered as a domain-decomposition technique and then show how the method can be adapted to solve the linear least squares problem $\min_x ||Ax - b||_2$. A global solution to this problem is determined by finding a set of local solutions with a specific linear combination of these local solutions determining the global update for the current iteration. Two-stage MS methods in which MS strategy is also applied to the individual systems of the MS, have also been considered for linear problems, I propose an alternative two-stage strategy in which the global updates of the MS are determined optimally. This does not exclude the former notion of two-stage MS. For the least-squares problem, the outer stage of the iteration can also be formulated as a least squares problem of dimension p, where p is the number of splittings in the MS. Theoretical results are presented which prove the convergence of the iterations. Numerical results which detail the iteration behavior relative to subproblem size, convergence criteria and recombination techniques are given. The two-stage MS strategy is shown to be effective for near-separable problems. The same strategy can also be applied for nonlinear optimization. In fact the proof of convergence for the least-squares problem relies on the theory for the general nonlinear case.

Organizer: Qing Nie

NOTE: The Postdoc Seminar is organized by the IMA postdoctoral members, but all interested IMA participants are very welcome to attend. The Seminar meets in Vincent Hall 570.

Wednesday, June 4

Special Postdoc Seminar in room Vincent Hall 570:

2:00 pm	**Ralf Hiptmair** University of Augsburg	Finite Elements for Differential Forms

Abstract: The mixed variational formulation of many elliptic boundary value problems involves vector valued function spaces, like, in three dimensions, $\mathbf{H}(\mathbf{curl}; \Omega)$ and $\mathbf{H}(\mathbf{div}; \Omega)$. Thus finite element subspaces of these function spaces are indispensable for meaningful finite element discretization schemes.

Given a simplicial triangulation of the computational domain Ω, among others, Raviart, Thomas and Nédélec have found suitable conforming finite elements for $\mathbf{H}(\mathbf{div}; \Omega)$ and $\mathbf{H}(\mathbf{curl}; \Omega)$ respectively. At first glance, it is hard to detect a common guiding principle behind these approaches. We take a fresh look at the construction of the finite spaces viewing them from the angle of differential forms. We exploit the well–known relationships between differential forms and differential operators: both **Div, curl** and **grad** can be regarded as special incarnations of the external derivative of a differential form. Moreover, in the realm of differential forms most concepts are basically dimension–independent.

Thus, we arrive at a fairly canonical procedure to construct conforming finite element subspaces of function spaces related to differential forms. In any dimension we can give a simple characterization of the local polynomial spaces and degrees of freedom making up the definition of the finite element spaces. With unprecedented ease we can recover the familiar $\mathbf{H}(\mathbf{div}; \Omega)$– and $\mathbf{H}(\mathbf{curl}; \Omega)$–conforming finite elements and establish the unisolvence of degrees of freedom. In addition, the use of differential forms makes it possible to establish crucial properties of the canonical interpolation operators and representation theorems in a single sweep for all kinds of spaces.

Thursday, June 5

Math Department Numerical Analysis Seminar in room Vincent Hall 570:

2:30 pm	**Lars Wahlbin** Cornell University	Stability, analyticity and almost best approximation for parabolic finite element equations

Friday, June 6

SEMINAR ON INDUSTRIAL PROBLEMS

11:15 am	**Tarek Habashy** Schlumberger-Doll Research	Application of Inverse Scattering to Oil Field Evaluation Problems

Abstract: In this presentation I will show some examples of the application of Inverse Scattering theory to oil-field evaluation problems. I will attempt to cover three applications (time permitting).

The first example is cross-well tomography. In this example, we introduce a novel approximation to numerically simulate the electromagnetic response in arbitrarily heterogeneous conductive media. The approximation is nonlinear with respect to the spatial variations of electrical conductivity. It introduces a source-independent scattering tensor whose projection on the background electric field (i.e. the electric field excited in the absence of conductivity variations) is an approximation to the electric field internal to the region of anomalous conductivity. This scattering tensor adjusts the background electric field by way of amplitude, phase and cross-polarization corrections that result from frequency-dependent mutual coupling effects among scatterers. In general, these three corrections are not possible with the more popular first-order Born approximation. As a result, the scattering tensor can accurately describe electromagnetic fields both inside and outside the region of anomalous conductivity in the presence of large contrasts in electrical conductivity as well as for large scatterer dimensions over a wide frequency range and, best of all, without losing the computational efficiency of a linear approximation, e.g., the Born approximation. We use this nonlinear scattering approximation in the inversion of cross-well data which allows the computation of an approximation to the Jacobian matrix needed in the implementation of a Gauss-Newton search approach. Several examples of cross-well inversion will be shown.

In the second example, I will present an inversion approach for reconstructing the electrical permittivity and conductivity of three-phase fluid mixtures flowing in a pipe. We have applied the inversion algorithm to the case where there are a number of antennas uniformly mounted on the surface of a pipe. Each antenna is a cross-dipole that provides two orthogonal polarizations: the circumferential and axial polarizations. For the reconstruction of the permittivity and conductivity maps from the measurement, we implemented an iterative procedure using a quasi Gauss-Newton method. In such a scheme the minimum of the objective or cost function is achieved through a line search along the steepest descent direction determined by the gradient of the cost function at the current iterate. The line search is implemented by computing an adjustable step-length along the search direction that always guarantees the reduction of the cost function from its value at the previous iterate. Finally, the values

of the permittivities and conductivities are constrained to be within their physical bounds. We present several examples where the reconstruction is performed using the amplitude and phase or the amplitude only.

In the third and last example, I will present an approach for imaging pits and holes in corroded steel casings. The measurement is based on magnetic flux leakage where a strong magnet creates a magnetic flux in the casing walls. The flux leakage sensors (Hall sensors) detect the fringing fields caused by casing defects which disturb the normal flux. Using analytical continuation of the flux leakage, a sharper image of pits can be reconstructed on the casing surface.

The seminar meets in the Seminar Room, Vincent Hall 570.

IMA Workshop:

Parallel Solution of PDE

June 9–13, 1997
Organizers: Mitchell Luskin (University of Minnesota) and
Petter Bjørstad (University of Bergen)

The numerical solution of the partial differential equations of continuum mechanics is of major importance to the development of many technologies and has been the target of much of the development of parallel computer hardware and software. Parallel computers offers the promise of greatly increased performance and the routine calculation of previously intractable problems. This workshop will promote the development and assessment of new approximation and solution techniques which can take advantage of parallel computers. Topics to be the focus of research include sparse matrix techniques, domain decomposition methods, parallel multi-grid methods, and novel time and space discretizations.

Monday, June 9

Talks today are in Lecture Hall EE/CS 3-180

8:30 am	**Registration and Coffee**	Reception Room EE/CS 3-176
9:00 am	**Welcome and Orientation**	A. Friedman, R. Gulliver, M. Luskin
9:15 am	**Xiao-Chuan Cai** University of Colorado	Overlapping Schwarz Methods and Applications in Compressible Flow Problems

Abstract: In this talk, we discuss some recent development of overlapping Schwarz methods (OSM), and then we focus on the application of OSM in the implicit solution of three-dimensional unsteady compressible Navier-Stokes equations discretized on moving unstructured meshes. Performance on distributed memory parallel computers will be reported.

10:05 am	**Rolf Rannacher** University of Heidelberg	A parallel multigrid solver for the incompressible Navier-Stokes equations

Abstract: The accurate solution of the incompressible Navier-Stokes equations requires high mesh resolution and very efficient algebraic solution strategies. The best overall efficiency can be obtained by using multigrid techniques which usually contain highly recursive components. This makes the effective parallelization of these methods difficult, as good parallel efficiency may strongly conflict with the goal of high numerical efficiency. We describe a multigrid-based Navier-Stokes solver which combines these two goals to a large extent. The algorithm uses operator splitting in the sense of the projection (or pressure correction) method where the inner linearized

problems are solved by multigrid iterations. The parallel efficiency is achieved by grid-blocking in the smoothing process without reducing the overall numerical efficiency too much.

10:50 am	**Coffee Break**	Reception Room EE/CS 3-176

11:15 am	**Paul F. Fischer** Brown University	An overlapping Schwarz method for spectral element solution of the incompressible Navier-Stokes equations

Abstract: We develop a finite element based additive Schwarz preconditioner for the spectral element formulation of the incompressible Navier-Stokes equations. The importance of the coarse grid solve in this context is demonstrated, and an efficient (direct) parallel coarse grid solver is presented which is particularly suited to large numbers of processors. For large two-dimensional problems this overlapping Schwarz approach can yield as much as a five-fold reduction in Navier-Stokes simulation time over previously employed methods based upon deflation.

2:00–2:20 pm	**Luca Pavarino** Università di Pavia	Overlapping Schwarz methods for saddle-point problems with a penalty term

Abstract: We introduce some parallel and scalable iterative methods for saddle-point problems with a penalty term, such as the mixed formulation of linear elasticity, the Stokes problem, and the linearized Navier-Stokes equations. These are domain decomposition methods of overlapping Schwarz type, based on the solution of local saddle point problems on overlapping subdomains and the solution of a coarse saddle point problem. The resulting indefinite preconditioner is accelerated by a Krylov space method such as GMRES. Numerical experiments indicate that the rate of convergence of the preconditioned operator is independent of the mesh size, the number of subdomains and the penalty parameter.

2:20–2:40 pm	**Guido Kanschat** University of Heidelberg	Parallel Solution of Radiative Transport Problems in Astrophysics

Abstract: Simulation of multidimensional radiative transfer problems is of high complexity. The domain of computation is 5-dimensional, making a combination of adaptive algorithms and parallel computation necessary for the solution. A method of distributing the ordinate space is presented. Linear systems are solved by Krylov-space methods combined with multi-level techniques. We avoid typical problems of parallel preconditioning of transport problems by a purely local preconditioner. A time complexity analysis will be presented, as well as two- and three-dimensional results.

2:40–3:00 pm	**Jie Shen** Penn State University	Fast Spectral-Galerkin Methods and its Applications

Abstract: We shall present in this talk some fast spectral-Galerkin algorithms developed in the last few years. Their computational complexities are comparable to those of finite difference and finite element algorithms, yet they provide much more accurate results while using a significantly smaller number of unknowns. Furthermore, the most computationally intensive components in these algorithms are matrix multiplications and/or fast Fourier transforms/fast multipole methods for which existing parallel software can be readily applied.

We shall also present recent numerical results using these fast spectral-Galerkin algorithms for various scientific and engineering applications, including computational fluid dynamics, atmosphere and oceanographic sciences and material sciences.

4:00 pm	**IMA Tea (and more!)**	Vincent Hall 502 (The IMA Lounge)

A variety of appetizers and beverages will be served.

Tuesday, June 10

Talks today are in Lecture Hall EE/CS 3-180

9:00 am	**Coffee**	Reception Room EE/CS 3-176
9:15 am	**Yvon Maday** Université Paris IV	To be announced
10:05 am	**Olof Widlund** Courant Institute, NYU	Some new domain decomposition methods for linear elasticity and Helmholtz's equation

Abstract: After an introduction, we consider the extension of iterative substructuring algorithms to the equations of linear elasticity. In order to be able to handle almost incompressible materials, we choose to work with mixed finite element methods; the resulting systems have much in common with finite element models for Stokes' equation. We explore a number of different algorithmic ideas, formulate new theoretical results, and report on some numerical experiments. Our work is joint with Luca Pavarino and principally concerns higher order methods of spectral element type.

In a second part, we discuss new domain decomposition algorithms for Helmholtz's equation. Our methods use overlapping subregions and the resulting local problems have boundary conditions of Sommerfeld type. Although the finite element approximation of the Helmholtz equation is continuous, the iterates can have jumps across the subdomain boundaries. Our algorithms generalizes a method developed and analyzed by Bruno Despres. Different variants are considered and results of numerical experiments are presented.

Our work is joint with Xiao-Chuan Cai, Mario Casarin, and Frank Elliott.

10:50 am	**Coffee Break**	Reception Room EE/CS 3-176
11:15 am	**Peter Bastian** University of Stuttgart	Parallel Multigrid Methods and Applications

Abstract: In my talk I will address several issues in the implementation of parallel multigrid methods on unstructured meshes. The basic algorithm can be used in two and three space dimensions and for many different discretization schemes and PDE systems. Dynamic load balancing schemes for additive and multiplicative multigrid in the case of adaptive local grid refinement will be presented. Since the implementation of all these methods requires a large programming effort a few remarks about the software design of the UG (Unstructured Grids) code are made. The flexibility of the code and its parallel and numerical efficiency are demonstrated for a large number of examples.

2:00–2:20	**Amir Averbuch** Tel Aviv University	Highly Scalable Two- and Three-Dimensional Navier-Stokes Parallel Solvers on MIMD Multiprocessors

Abstract: We present a new parallel algorithm for the solution of the incompressible two- and three-dimensional Navier-Stokes equations. The parallelization is achieved via domain decomposition. The computational region is considered in the form of a 2-D or 3-D periodic box decomposed into parallel strips (slabs). For time discretization we use a third order multistep method. The time discretization procedure results in solving global elliptic problems of (monotonic) Helmholtz and Poisson types in each time step. For the space discretization we employ the multidomain local Fourier (MDLF) method. The discretization in the periodic directions is performed by the standard Fourier method. In the direction across the strips we use the Local Fourier Basis technique which involves the overlapping of the neighboring subdomains and smoothing of local functions across the interior boundaries (interfaces). The matching of the local solutions is performed by adding properly weighted interface Green's functions. Their amplitudes are found in terms of the jumps of the solution and its first derivatives at the interfaces.

Without the pressure term in each time step only the Helmholtz type equations were solved. It was shown that the parallel solution of this equation can be accomplished using only local (neighbor-to-neighbor) communication due to localization properies of the Helmholtz operator.

We here consider the complete Navier-Stokes system including the pressure term. The solution of the Poisson equation for pressure has the potential to degrade the performance and the achieved speedup of a parallel algorithm due to the global nature of this equation that necessitates global communication among the processors.

However, we show that only a few lowest harmonics require the global data trasfer whereas the rest of harmonics can be treated locally. Therefore, most of the communication that is required for parallelization of the Navier-Stokes solver using the MDLF method is mainly local between adjacent subdomains (processors). Moreover, the percentage of the time spent in global communication reduces as the size of the problem increases. Thus, the present parallel algorithm is highly scalable.

The 2-D and 3-D Navier-Stokes solvers are implemented on three MIMD message-passing multiprocessors (a 60-processors IBM SP2, a 20-processors MOSIX, and a network of 10 Alpha workstations) and achieve an efficiency of more than 70with the PVM (parallel virtual machine) software package was executed on all the above distinct computational platforms.

This is joint work with L. Vozovoi, M. Israeli and L. Ioffe.

2:20–2:40	**Ralf Hiptmair** University of Augsburg	Multigrid Method for Maxwell's Equations

Abstract: The problem under consideration is the wave equation for the electric field in a 3D cavity with perfectly conducting walls. When treated in the time domain an implicit timestepping is highly desirable due to its unconditional stability. In a finite-element setting each timestep involves the solution of a discrete variational problem for the bilinear form $(\cdot,\cdot)_0 + (\mathbf{curl}\cdot, \mathbf{curl}\cdot)_0$ posed over $\mathbf{H(curl;}\ \Omega\mathbf{)}$. I relied on Nedelec's $\mathbf{H(curl;}$ $\Omega\mathbf{)}$-conforming finite elements (edge elements), which yield a viable discretization for Maxwell's equations.

A multigrid method is employed as a fast iterative solution method. Since proper ellipticity of the bilinear form is confined to the complement of the kernel of the **curl**–operator, discrete Helmholtz–decompositions of the finite element spaces are crucial for the design and analysis of the multigrid scheme.

Under certain assumptions on the computational domain and material functions, a rigorous proof of asymptotic optimality of the multigrid method can be given; it shows that convergence does not deteriorate on very fine grids. The results of numerical experiments confirm the practical efficiency of the method.

2:40–3:00 pm	**Andrea Toselli** Courant Institute, NYU	Overlapping Schwarz methods for Maxwell's equations in three dimensions

Abstract: Overlapping methods Schwarz are considered for finite element problems of 3D Maxwell's equations. Né délec elements built on tetrahedra and cubes are considered. Once the relative overlap is fixed, the condition number of the additive Schwarz method is bounded, independently of the diameter of the triangulation and the number of subregions. A similar result is obtained for a multiplicative method. Our work generalizes well-known results for conforming finite elements for second order elliptic scalar equations.

Wednesday, June 11

Talks today are in Lecture Hall EE/CS 3-180

9:00 am	**Coffee**	Reception Room EE/CS 3-176
9:15 am	**Jinchao Xu** Penn State University	Multigrid methods for solving partial differential equations discretized with unstructured grids

Abstract: A number of techniques will be discussed in this talk on how a finite element equation posed on an unstructured grid in two or three dimensions can be solved within optimal computational complexity by special multigrid methods such as nonnested multigrid methods, agglomeration methods and auxiliary space methods. Certain ellipic (and parabolic) problems including convection dominated equations will be discussed as examples.

10:05 am	**Maksymilian Dryja** Warsaw University	An additive Schwarz method for finite-element anisotropic elliptic problems

Abstract: A finite-element approximation of anisotropic second order elliptic problems on a region, which is a

union of rectangles, is discussed. The coefficients are piecewise constant on rectangular subregions of the original region. The additive Schwarz method (AMS) with minimal overlap for solving the resulting systems is described and analyzed. It uses three coarse spaces, standard and two special.

A rate of convergence of the method is of the order of $(H/h)^{\frac{1}{2}}$ when cg is used. Here H and h are parameters of the coarse and fine triangulation. The rate of convergence of the method is independent of the coefficients, i.e. their discontinuity and anisotropy.

This is joint work with Petter Bjørstad.

10:50 am	**Coffee Break**	Reception Room EE/CS 3-176
11:15 am	**Bjørn Engquist** Univ. of California, Los Angeles	Large-scale simulations of hyperbolic problems

Abstract: The speed of propagation in hyperbolic partial differential equations is finite. This means that explicit methods are natural in many cases. Spatial data distribution and the corresponding parallel algorithms are then often straightforward. We shall discuss efficiency of such algorithms but also present problems for which this simple setting is not optimal. Applications to fluid mechanics and electromagnetics will be considered.

2:00–2:20 pm	**Tsorng-Whay Pan** University of Houston	A Lagrange multiplier/fictitious domain method for particulate flows

Abstract: We would like to discuss the application of a Lagrange multiplier based fictitious domain method to the numerical simulation of incompressible viscous flow modelled by the Navier-Stokes equations around moving bodies. The solution method combines finite element approximations, time discretization by operator splitting and conjugate gradient algorithms for the solution of the linearly constrained quadratic minimization problems coming from the splitting method. The advantage of fictitious domain techniques is that we can use uniform structured mesh and hence fast solvers (future plans to use parallel solvers will be discussed). The results of numerical experiments for 100 sedimenting cylinders in a two-dimensional channel will be presented.

2:20–2:40 pm	**Marian Vajtersic** Slovak Academy of Sciences	A Semidirect Biharmonic Solver for VLSI

Abstract: An efficient VLSI algorithm for solving the model biharmonic problem will be presented. The complexity of this VLSI solver will be characterized in terms of the area $\times$ time measure AT^2, where A and T stand respectively for the *time* and the *area* required for the parallel algorithm.

The first boundary value problem for the biharmonic equation will be considered for a rectangular domain with $n \times n$ interior grid points. The VLSI algorithm is based on the semidirect approach which treats the biharmonic operator as a coupled pair of Laplace operators.

The design is of a compact form where one VLSI block performs all operations of the semidirect cycle. Its length and height are proportional to $O(n \log n)$. The total parallel computational time is $O(\sqrt{n} \log^2 n)$. Hence, the global estimation in AT^2 complexity measure is $O(n^3 \log^6 n)$ for this algorithm. This represents the best AT^2 upper bound for the biharmonic problem until now.

2:40–3:00 pm	**Barry Smith** Argonne National Laboratories	Parallel Newton-Krylov-Schwarz methods: Implementation Issues

Abstract: I will discuss several specific issues in the implementation of parallel Newton-Krylov-Schwarz methods with general-purpose numerical libraries for the solution of PDEs.

This is joint work with Dinesh Kaushik and David Keyes.

Thursday, June 12

Talks today are in Lecture Hall EE/CS 3-180

9:00 am	**Coffee**	Reception Room EE/CS 3-176
9:15 am	**Ronald H. W. Hoppe** University of Augsburg	Adaptive finite element methods for domain decomposition on nonmatching grids

Abstract: We consider the parallel solution of elliptic boundary value problems discretized by domain decomposition methods on nonmatching grids involving mortar finite elements. We start from an initial nonoverlapping decomposition of the computational domain and independent triangulations of the subdomains realizing weak continuity conditions on the internal subdomain boundaries by means of appropriately chosen Lagrangean multipliers. The solution process features a preconditioned Lanczos iteration for the resulting saddle point problem using a block diagonal preconditioner and an adaptive local mesh refinement on the basis of residual based or hierarchical a posteriori error estimators.

In the parallel implementation of the code, the data related to the subdomains are appropriately distributed among the available processors.

The efficiency of the parallel implementation and the adaptive grid refinement process is illustrated by numerical simulation results obtained on a IBM SP2 for some selected test problems including potential flow around profiles.

This is joint work with Yu. Vassilevski and B. Wohlmuth.

10:05 am	**Tony Chan** Univ. of California, Los Angeles	Algebraic nonoverlapping domain decomposition methods for compressible fluid flow problems on unstructured meshes

Abstract: We consider preconditioning methods for convection-dominated fluid flow problems based on a nonoverlapping Schur complement domain decomposition procedure for arbitrary triangulated domains. The triangulation is first partitioned into a number of subdomains and interfaces which induce a natural 2×2 partitioning of the p.d.e. discretization matrix. We view the Schur complement induced by this partitioning as an algebraically derived coarse space approximation. This avoids the known difficulties associated with the direct formation of an effective coarse discretization for advection dominated equations. By considering various approximations of the block factorization of the 2×2 system, we have developed a family of robust preconditioning techniques.

These approximations are introduced to improve both the sequential and parallel efficiency of the method without significantly degrading the quality of the preconditioner. The specific approximations that we have used include ILU-preconditioned GMRES subdomain solves, localized approximation of the interface Schur complement, and limited level-fill ILU interface backsolves. A computer code based on these ideas has been developed and tested on the IBM SP2 using MPI message passing protocol. A number of 2-D CFD calculations will be presented for both scalar advection-diffusion equations and the Euler equations. These results show very good scalability of the preconditioner as the number of processors is increased while the number of degrees of freedom per processor is fixed.

This is joint work with Tim Barth and Wei-Pei Tang.

10:50 am	**Coffee Break**	Reception Room EE/CS 3-176
11:15–11:45	**Viswanathan Babu** Ford Scientific Research Lab.	Simulation of Incompressible Flows Using the Lattice Boltzmann Method

Abstract: The lattice Boltzmann (LB) method, which is closely related to the lattice gas (LG) method, will be discussed in detail. The LG method is boolean in nature using only bits to indicate the presence or absence of a particle moving in a particular direction and speed. The absence of floating point operations gives the LG method unconditional numerical stability but restricts it to specialized hardware that can perform the Boolean logical operations efficiently. The Boolean character also results in a noisy signal that must be averaged over space/time for reliable estimates. The LB method, on the other hand, tracks the distribution functions (or time averages) of the particles. As a result, floating-point numbers have to be used and so the method is not boolean. While this makes the LB method susceptible to instabilities due to accumulation of round-off errors, it allows the LB method to use a variety of existing computer platforms. The signal-to-noise ratio of the LB method is also significantly higher than the LG method. Both the LB method and the LG method are highly parallel. In fact, the LB method optimizes extremely well on current computer platforms as will be demonstrated in this talk. The current version of the LB code developed at FRL runs at speeds around 1.7 Gflops (2D code) and 2.0 Gflops (3D code) on a 32 processor Cray T3D. The 3D code has super-linear speedup (linear being the theoretical maximum) and runs at a speed of 33 Gflops on a 512 processor T3D.

The objective of this talk is to demonstrate the potential of this method as a viable tool for performing time accurate simulations of incompressible flows. To that end, two issues will be examined in detail — accuracy and speed. The spatial and temporal accuracy of the LB method will be established through suitable benchmark studies. It is important to note here that the method is formally second-order accurate in both space and time, an accuracy that exceeds that of many commercial codes today. The speed at which the code runs will be demonstrated through actual production runs on the parallel Cray T3D. As an example of the phenomenal performance of the LB code developed at FRL, consider the following fact. Each processor on the T3D has a read bandwidth from memory to cache that is limited to 320 Mbytes/sec, which translates to 40 Mflops since the T3D is a 64 bit machine (8 bytes/word). Codes that do not have cache reuse will be hardware limited to this speed. Our code runs at a speed of 60 Mflops on this processor through cache reuse and other optimizations.

This is joint work with Gary S. Strumolo.

11:45-12:05 pm	**Kenneth H. Karlsen** University of Bergen	Front Tracking and Corrected Operator Splitting for Advection-Diffusion Problems

Abstract: We give a brief overview of a numerical method for advection dominated advection-diffusion problems based on combining, via a dynamical equation splitting, a front tracking method for conservation laws with a finite element method for parabolic equations.

This is joint work with Helge K. Dahle, Knut-Andreas Lie, and Nils Henrik Risebro.

6:00 pm	**Workshop Dinner** Radisson Hotel	Alumni Room, second floor

Reception at 6:00 in the Alumni Room, dinner at 6:30.

Friday, June 13

Talks today are in Lecture Hall EE/CS 3-180

9:00 am	**Coffee**	Reception Room EE/CS 3-176
9:15 am	**Hans Munthe-Kaas** University of Bergen	Coordinate-free methods in scientific computing

Abstract: The basic philosophy behind object-oriented program design is that programming consists of two distinct parts, 'WHAT' and 'HOW'. The WHAT part is defining the functionality and interraction between software modules (classes), while the HOW part provides algorithms and datastructures which are hidden within the class.

The main difference between the treatment of differential equations in pure and applied mathematics is that applied mathematics is being developed and presented in terms of concrete representations (i.e. specific coordinate systems), while pure mathematics has been more concerned with those properties of the mathematical objects which are independent of particular coordinate systems. Hence, it has been necessary to develop tools and languages for discussing differential equations in a coordinate-free setting.

Motivated by the needs of telling WHAT without telling HOW in object-oriented programming, we have for several years been investigating what we can benefit by using the tools and concepts of pure mathematics in scientific computing. This has recently led to significant new insights and new algorithms. The first major insight we gained by this approach was a new approach to tensor computations using the language of category theory. This approach has several advantages compared to the more familiar index-based approach to tensor computations. In particular the category-theoretical approach leads to much simpler computer programs for dealing with symmetries. More recently, we have studied numerical time integration of differential equations in a coordinate-free setting. This has lead to new algorithms based on Lie group actions on manifolds, and has now become a very active field of research.

In this talk we will give an introduction to this line of work, and discuss one of the topics in somewhat more detail.

10:05 am	**David E. Keyes** Old Dominion Univ. & ICASE	Think Globally, Act Locally: Newton-Krylov-Schwarz Algorithms for Parallel CFD

Abstract: Newton-Krylov methods and Krylov-Schwarz (domain decomposition) methods have begun to become established in computational fluid dynamics (CFD) over the past decade. The former employ a Krylov method, such as the generalized minimal residual method, inside of Newton's method in a Jacobian-free manner, through directional differencing. The latter employ overlapping Schwarz-type decomposition to derive a preconditioner for the Krylov accelerator that relies primarily on local information, for parallelism. They may be composed as Newton-Krylov-Schwarz methods, which seem particularly well suited for solving nonlinear elliptic systems in high-latency distributed-memory environments.

We describe recent numerical simulations with Newton-Krylov-Schwarz methods in CFD carried out at ICASE/NASA Langley, emphasizing trade-offs in convergence rate and concurrency in implicit algorithms, the preconditioning of a higher-order discrete operator with a lower-order discrete operator, and comparisons with multigrid and standard defect-correction approaches. We also present recent results on globalization through pseudo-transient continuation and additive Schwarz for convectively dominated problems.

10:50 am	**Coffee Break**	Reception Room EE/CS 3-176
11:15 am	**Susanne Brenner** Univ. of South Carolina	Domain decomposition for nonconforming plate elements

Abstract: The simplest plate elements are nonconforming, but the domain decomposition theory developed for conforming finite elements are not directly applicable to them. The complications due to the nonconformity of these elements can be overcome by exploiting their "conforming relatives". In this talk we will present results on the two-level additive Schwarz method (overlapping) and the balanced domain decomposition method (nonoverlapping) for nonconforming plate elements.

Monday, June 16

Tuesday, June 17

IMA Postdoc Seminar

2:30 pm	**Hans D. Mittelmann** Arizona State University	Computational Results for Capillary Surfaces: or, Where is the Liquid in a Cube?

Abstract: The topic is the distribution of liquid inside a cube for zero or moderate gravity and various contact angles. In the zero-gravity case additional symmetry requirements are imposed. A number of interesting and some surprising solutions are obtained and a classification is attempted. Finally, it is investigated what happens when the contact angles along walls meeting in a corner are different.

Organizer: Qing Nie

NOTE: The Postdoc Seminar is organized by the IMA postdoctoral members, but all interested IMA participants are very welcome to attend. The Seminar meets in Vincent Hall 570.

Wednesday, June 18

IMA Industrial Postdoc Seminar

The seminar will meet from 1:00 – 4:30 pm today in Vincent Hall 570. The format of the seminar is:

1. Presentation of projects and problems from industry (Honeywell, Lockheed Martin and Kodak) on which the industrial postdocs are working.
2. Informal suggestions and discussion among the participants.

The seminar is directed by Avner Friedman and Walter Littman. Visitors who plan to attend are requested to inform Dr. Friedman.

Thursday, June 19

Math Department Numerical Analysis Seminar in room Vincent Hall 570:

1:30 pm	**Endre Suli** Oxford University	A-posteriori error analysis and adaptivity for finite element approximations of hyperbolic problems

IMA Picnic

The picnic will be at the Dome Shelter in Como Park, St. Paul, near the Como Zoo. The picnic begins at 4:00 pm, with dinner served at 5:00 pm. IMA staff, postdocs and visitors and their families are encouraged to come!

Friday, June 20

Monday, June 23

IMA Postdoc Seminar

2:30 pm	**Jeff Derby** University of Minnesota	Materials Processing Simulations via High-Performance Computing

Abstract: Advanced materials are used in a wide variety of systems which rely on new materials for their novel mechanical, electronic, or optical properties. Computational materials research brings the tools of modern high-performance computing to bear upon issues in both the design and processing of advanced materials. This approach promises to complement and extend the traditional paradigm of experimental investigation, thereby accelerating the development of new materials and the optimization of processes used to produce existing materials.

With the continuing advance of parallel computer hardware and appropriate algorithms, high-performance computing coupled with mathematical modeling has proven to be an increasingly useful approach for understanding the processing of materials. These processes are typically characterized by complicated nonlinear interactions between field and interfacial phenomena, specifically the transport of momentum, heat, and mass, and often coupled with solidification, growth kinetics, capillarity, and interface morphology.

We have developed a suite of modeling tools which are based on the finite element method and implemented on various high performance computing platforms, ranging from the Cray C-90, a vector machine, to the Thinking Machines Corporation CM-5 and the Cray T3D, both massively parallel supercomputers. In this presentation, the most salient features of these models will be highlighted and results will be presented from their application to describe fluid flows in a number of materials processing situations, including the growth of large single crystals of electronic and photonic materials, the viscous sintering of glassy ceramic particles, and the shear-induced break-up of fluid drops immersed in an immiscible polymeric liquid.

Organizer: Qing Nie

NOTE: The Postdoc Seminar is organized by the IMA postdoctoral members, but all interested IMA participants are very welcome to attend. The Seminar meets in Vincent Hall 570.

Tuesday, June 24

Wednesday, June 25

Thursday, June 26

Friday, June 27

Sunday, June 29

Workshop on Automatic Differentiation for Large-Scale Applications begins (June 29–July 3).

Monday, June 30

CURRENT IMA PARTICIPANTS

POSTDOCTORAL MEMBERS FOR 1996–97 PROGRAM YEAR

NAME	PREVIOUS INSTITUTION
GOBBERT, MATTHIAS	Arizona State University
LOTOTSKY, SERGEY	University of Southern California
MALIASSOV, SERGUEI	Texas A&M University
NGUYEN, BRIAN	University of Michigan
NIE, QING	Ohio State University
SARKAR, SANHITA	University of Minnesota
SUCHOMEL, BRIAN	University of Wyoming
YANG, DAOQI	Wayne State University

POSTDOCTORAL MEMBERSHIPS IN INDUSTRIAL MATHEMATICS FOR 1996–97

NAME	PREVIOUS INSTITUTION	INDUSTRIAL AFFILIATION
CHAWLA, SANJAY	University of Tennessee	Honeywell
KOURITZIN, MICHAEL	Carleton University	Lockheed Martin
LOPEZ, GILBERTO	Northwestern University	Eastman Kodak
WANG, LEI	University of Washington	Honeywell

VISITORS IN RESIDENCE (as of 5/21)

AVERBUCH, AMIR	Tel Aviv University	JUN 6 - 13
BABU, VISWANATHAN	Ford Motor Company	JUN 8 - 13
BASTIAN, PETER	University of Stuttgart	MAY 14 - JUN 13
BIELAK, JACOBO	Carnegie Mellon University	JUN 8 - 13
BJØRSTAD, PETTER	University of Bergen	SEP 1 - JUN 30
BORUCKI, LEN	Motorola Inc.	JUN 26 - 27
BRENNER, SUSANNE	University of South Carolina	JAN 13 - JUN 30
BROWN, STEPHEN	University of Hertfordshire	JUN 27 - JUL 3
BURNS, JOHN	Virginia Polytechnic & State Univ.	JUN 27 - JUL 3
CAI, XIAO-CHUAN	University of Colorado	JUN 8 - 13
CARLE, ALAN	Rice University	JUN 27 - JUL 3
CASTILLO-CHAVEZ, CARLOS	Cornell University	JUN 15 - 16
CASTRO, PETER	Eastman Kodak	JUN 26 - 27
CHAN, TONY F.C.	Univ. of California-Los Angeles	JUN 8 - 13
CHARPENTIER, ISABELLE	Lab. de Model. et Calc. Grenoble	JUN 27 - JUL 3

CHENEY, MARGARET	Rensselaer Polytechnic Institute	JAN 1 - JUN 30
CHOCK, DAVID	Ford Motor Company	JUN 26 - 27
COCKBURN, BERNARDO	University of Minnesota	SEP 1 - AUG 31
COLEMAN, THOMAS	Cornell University	JUN 29 - JUL 2
COWSAR, LAWRENCE C.	AT&T Bell Laboratories	JUN 7 - 13
DE PILLIS, LISETTE	Harvey Mudd College	JUN 8 - 13
DOBSON, DAVID	Texas A&M University	JUN 27 - JUL 3
DRYJA, MAX	Warsaw University	MAY 19 - JUN 19
ENGQUIST, BJORN	Univ. of California-Los Angeles	JUN 8 - 13
FAURE, CHRISTELE	INRIA Sophia Antipolis	JUN 28 - JUL 3
FENG, XIAOBING	University of Tennessee	APR 1 - JUN 30
FISCHER, PAUL F.	Brown University	JUN 1 - 30
FLAHERTY, JOSEPH	Rensselaer Polytechnic Institute	APR 1 - JUN 30
FRIEDMAN, AVNER	Institute for Mathematics	SEP 1 - AUG 31
GARRETT, DAVID	Lockheed Martin	JUN 27 - 27
GEISLER, CHARLES	Minnesota Technology Incorp.	JUN 27 - 27
GIERING, RALF	Max-Planck-Inst. für Meteor., Hamburg	JUN 27 - JUL 3
GILG, ALBERT	Siemens AG, Munich	JUN 26 - 27
GOLDMAN, VICTOR	University of Twente	JUN 27 - JUL 3
GREENSIDE, HENRY	Duke University	JUN 9 - 13
GUCKENHEIMER, JOHN	Cornell University	JUN 27 - JUL 3
GULLIVER, ROBERT	Institute for Mathematics	SEP 1 - AUG 31
HABASHY, TAREK M.	Schlumberger-Doll Research	JUN 5 - 6
HEINKENSCHLOSS, MATTHIAS	Rice University	JUN 27 - JUL 3
HEJHAL, DENNIS	University of Minnesota	SEP 1 - AUG 31
HIPTMAIR, RALF	Universität Augsburg	MAY 31 - JUN 15
HOPPE, RONALD H. W.	University of Augsburg	JUN 1 - 30
KANSCHAT, GUIDO	University of Heidelberg	MAY 29 - JUN 29
KARLSEN, KENNETH H.	University of Bergen	MAY 14 - JUN 15
KEYES, DAVID E.	ODU/ICASE	JUN 1 - 21
KIRSCHNER, DENISE	Univ. of Michigan Medical School	JUN 15 - 16
KRUZIK, MARTIN	Czech Academy of Sciences	SEP 1 - JUN 30
KUBOTA, KOICHI	Chuo University	JUN 27 - JUL 3
LIANG, JIE	University of Illinois at Urbana	JUN 29 - 30
LITTMAN, WALTER	University of Minnesota	SEP 1 - AUG 31
LOWENGRUB, JOHN	University of Minnesota	SEP 1 - AUG 31
LUCAS, ROH	Argonne National Labs	JUN 27 - JUL 3
LUSKIN, MITCHELL	University of Minnesota	SEP 1 - AUG 31
MADAY, YVON	Université Paris IV	JUN 8 - 13
MANKE, JOE	Boeing Info. & Support Services	JUN 28 - JUL 3
MARIN, SAM	General Motors Research Labs	JUN 26 - 27
MCKENNA, JAMES	Bellcore Communications Research	JUN 26 - 27
MISEMER, DAVID	3M General Offices	JUN 27 - 27
MITTELMANN, HANS	Arizona State University	JUN 8 - 20
MUNTHE-KAAS, HANS	Cambridge University	JUN 1 - 30
NAUMANN, UWE	Barbican YMCA	JUN 27 - JUL 3
NEUHAUSER, CLAUDIA	University of Minnesota	JUN 15 - 16
NUMRICH, ROBERT	Cray Research	JUN 27 - 27
PAN, TSORNG-WHAY	University of Houston	JUN 8 - 13
PAVARINO, LUCA	Università di Pavia	MAY 21 - JUN 19
PETZOLD, LINDA	University of Minnesota	JUN 27 - JUL 3
POLING, T. CRAIG	Lockheed Martin	JUN 27 - 27
PROHL, ANDREAS	Universität Heidelberg	SEP 1 - JUN 30
PULLEYBLANK, WILLIAM	IBM T.J. Watson Research Center	JUN 26 - 27
RACKNER, BARRY	Minnesota Supercomputer Center	SEP 1 - AUG 31
RAHMAN, TALAL	University of Bergen	MAR 11 - JUN 20

RANNACHER, ROLF	University of Heidelberg	APR 2 - JUN 23
RENAUT, ROSEMARY	Arizona State University	MAY 11 - JUN 14
ROH, LUCAS	Argonne National Labs	JUN 27 - JUL 1
ROKYTA, MIRKO	Charles University, Prague	JUN 8 - 13
RUDIN, BERNARD	IBM	JUN 26 - 27
SCAPOLLA, TERENZIO	Università di Pavia	JUN 8 - 13
SELL, GEORGE	University of Minnesota	SEP 1 - AUG 31
SHAPIRA, YAIR	Los Alamos National Laboratory	JUN 8 - 15
SHU, CHI-WANG	Brown University	APR 1 - JUN 30
SMITH, BARRY F.	Argonne National Laboratories	JUN 8 - 13
STEIN, GUNTER	Honeywell	JUN 27 - 27
SULI, ENDRE	Oxford Univ. Computing Laboratory	JUN 1 - 30
ŠVERÁK, VLADIMIR	University of Minnesota	SEP 1 - AUG 31
SYMES, WILLIAM	Rice University	JUN 27 - JUL 3
TAGO, YOSHIO	Fujitsu Limited	JUN 26 - 27
TALAGRAND, OLIVIER	École Normale Superieure	JUN 27 - JUL 3
TOSELLI, ANDREA	New York Univ.-Courant Institute	JUN 8 - 13
TURNER, WESLEY	Rensselaer Polytechnic Institute	JUN 8 - 13
UTKE, JEAN	Argonne National Laboratory	JUN 28 - 29
VAJTERSIC, MARIAN	Slovak Academy of Sciences	MAY 29 - JUN 15
VAN DEN DRIESSCHE, PAULINE	University of Victoria	JUN 15 - 16
VERMA, ARUN	Cornell University	JUN 27 - JUL 3
VERWER, JAN G.	CWI, Amsterdam	JUN 8 - 13
WAHLBIN, LARS B.	Cornell University	MAY 31 - JUN 7
WIDLUND, OLOF B.	New York Univ.-Courant Institute	JUN 7 - 13
WILDBERGER, MARTIN	EPRI	JUN 26 - 27
XIE, DEXUAN	New York University	JUN 8 - 13
XU, JINCHAO	Pennsylvania State University	JUN 8 - 18
ZHANG, CHAOMING	Rice University	JUN 27 - JUL 3
ZHANG, JUN	University of Minnesota	JUN 9 - 13
ZHAO, JENNIFER	Univ. of Michigan-Dearborn	JUN 2 - 30